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**EXPLICIT ROBUST SCHEMES FOR IMPLEMENTATION OF A CLASS OF
PRINCIPAL VALUE-BASED CONSTITUTIVE MODELS:
THEORETICAL DEVELOPMENT**

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ABSTRACT

The issue of developing effective and robust schemes to implement a class of the Ogden-type hyperelastic constitutive models is addressed. To this end, explicit forms for the corresponding material tangent stiffness tensors are developed, and these are valid for the entire deformation range; i.e., with both distinct as well as repeated principal-stretch values. Throughout the analysis the various implications of the underlying property of separability of the strain-energy functions are exploited, thus leading to compact final forms of the tensor expressions. In particular, this facilitated the treatment of complex cases of uncoupled volumetric/deviatoric formulations for incompressible materials. The forms derived are also amenable for use with symbolic-manipulation packages for systematic code generation.

1. INTRODUCTION

To a large extent, constitutive models of the so-called generalized Rivlin-Mooney type [1,2]; i.e., with the (stored) strain energy density written as a polynomial function in terms of the deformation *invariants*, have dominated the phenomenological theory of isotropic hyperelasticity [1-6], as well as the related *computational* literature on *finite-strain* elasticity [7-9], over the years. Recently, alternative representations in terms of the principal stretches have become increasingly popular in nonlinear finite element analyses [6,8,13]. In particular, several forms in this category were given by Ogden [5], Peng [11], and Valanis and Landel [12]. From both the mathematical and physical standpoints, these latter models exhibit a number of attractive features. For instance, in the *Valanis-Landel hypothesis* [12], also called the *separability* assumption, the underlying their mathematical structure (i.e., a strain energy depending on separate symmetric functions in each of the principal stretches) was found to be essential for effective and accurate characterization of the behavior of incompressible, and slightly-compressible, rubbers at (relatively) high strain levels [5,6].

However, from the viewpoint of numerical implementation, the use of these models presents a number of unique and difficult problems, which do not arise in alternative representations in terms of the strain invariants. Basically, the main difficulty here stems from the fact that, in addition to their being "reasonably complicated" functions of the strain components, the orthonormal basis of *eigenvectors* associated with the principal stretches (eigenvalues) are not uniquely defined for the whole deformation spectrum; i.e., *nonuniqueness* for the case of two or three *repeated* eigenvalues [14,16-18]. This will be a major source of difficulty in obtaining the (directional) derivative of the tensor-valued stress function (in terms of deformation tensor) needed to obtain the elastic-moduli matrix (i.e., material *tangent stiffness*). These latter arrays are essential ingredients in any nonlinear incremental finite element solution; e.g. using either the total *Lagrangian*, or *Eulerian* or "updated" Lagrange approaches [8,20]. General solutions of this type will typically involve very complex, nonproportional deformation paths during which the number of uniquely-defined eigenvectors will change, and the necessity of obtaining explicit forms for the material stiffness in such *singular* or *limiting* cases becomes obvious.

The type of problem mentioned above is not new; it has a long standing in various applications in continuum mechanics [21-28]. An important case to the point concerns the use of Hencky-type, or logarithmic strain measures in various contexts [25,27]; e.g. in conjunction with derivations of alternative forms for its (material) time derivative [22,24], the associated conjugate stresses [25], the so-called Hill's principal-axes techniques in the numerical treatment in [26], etc. However, to the present authors' knowledge, the topic has not been previously addressed in the context of deriving material-moduli tensors, for the general *three-dimensional* analysis. For suitable particular forms in the case of two repeated eigenvalues, but restricted to the *two-dimensional* problem, we refer to [8,13] for simple derivations.

Addressing the above problem constitutes the main objective in the present paper. In particular, we give details leading to the derivation of the proper *explicit* forms for the stress-deformation relationships, and the associated material elasticity arrays, in terms of general components of the deformation tensor for the entire regime of *distinct* as well as repeated; i.e., *double* or *triple* coalescence, eigenvalues of the strain tensor. In this, two specific forms of the Ogden-type strain-energy functions are considered; these are of sufficient generality to include most (if not all) of the models currently in common use. The first form is for the so-called general, unconstrained, materials using the traditional definition of principal stretches. The second is suitable for treating incompressible, and slightly compressible, cases and it makes use of a *modified* set of principal stretches. These are associated with the concept of deformation *decomposition* into pure *dilation-isochoric distortion* response components, which has been utilized extensively in recent literature [5,8,9,13], including works on finite elastoplasticity [9,10]. For both of these models the implications of the underlying separable property are exploited throughout the derivation, thus providing a convenient means for performing the limiting process. For instance, this eliminates the need for a

posteriori search and identification of various "singular" expressions that may (appropriately) combine to give nonzero limits in scalar/tensor-valued *composite* terms [8,13].

2. PRELIMINARIES

For convenience, we summarize in this section some fundamentals and results pertinent to the large-deformation analysis. These will be referred to repeatedly in subsequent discussions and derivations. Here, and for the remainder of the paper, both indicial and the "counterpart" matrix notations will be used interchangeably; repeated indices imply the summation convention. Only rectangular Cartesian coordinate systems are employed, and we use lower-case subscripts for all tensor indices. For the most part, this is sufficient for our purpose here, and there is no need to consider lowering or raising of indices. Note, however, that the only exception to this concerns the definitions of "pull-back" and "push-forward" of tensors given below.

2.1 Basic-Kinematics

In line with common usage [e.g. 14-16], the set-up used to describe the nonlinear kinematics of a continuum is as follows. Let P be a material point with position vector \mathbf{X} in the undeformed (initial) configuration "B". The map of P in the (current) deformed configuration "b" is denoted by p whose location is given by \mathbf{x} . The deformation map is defined by $\phi: B \rightarrow b$, and

$$\mathbf{x} = \phi(\mathbf{X}, t) \quad ; \quad \mathbf{F} = \partial \phi / \partial \mathbf{X} \quad (\text{or } F_{ij} = \partial \phi_i / \partial X_j) \quad (2.1)$$

where \mathbf{F} is the (two-point) *deformation gradient* tensor for the current configuration "b" (at time t). Because of the one-to-one nature of the deformation map, \mathbf{F} is nonsingular and it can thus be expressed as follows, using the (right) polar-decomposition theorem,

$$\mathbf{F} = \mathbf{R} \mathbf{U} \quad ; \quad \text{or } F_{ij} = R_{ik} U_{kj} \quad (2.2)$$

where \mathbf{U} is the symmetric, positive definite, *pure stretch tensor*, and \mathbf{R} is a (proper-orthogonal) *rigid-rotation* tensor, such that

$$\mathbf{R} \mathbf{R}^T = \mathbf{I} \quad ; \quad \mathbf{C} = \mathbf{U}^2 = \mathbf{F}^T \mathbf{F} \quad ; \quad J = \det \mathbf{U} = \det \mathbf{F} \quad (2.3)$$

where \mathbf{I} is the second-order identity tensor, the superscript "T" indicates a transpose, and \mathbf{C} is known as the (right) Cauchy-Green *deformation* tensor and J represents the change in volume.

Through eqs. (2.1)-(2.3), several other strain measures can be defined. For example, we recall here the following familiar expressions for Green-Lagrange strain, \mathbf{E} , and Almansi strain, \mathbf{e} , respectively,

$$\mathbf{E} = \frac{1}{2}(\mathbf{C} - \mathbf{I}) \quad (2.4)$$

$$\mathbf{e} = \frac{1}{2}(\mathbf{I} - \mathbf{F}^{-T} \mathbf{F}^{-1}) \quad (2.5)$$

where $(\)^{-1}$ indicates an inverse. These are *material* and *spatial* strain fields [Sec. 2.2], respectively.

As an alternative to Eq. (2.2), we may employ the following decomposition for \mathbf{F} :

$$\mathbf{F} = J^{1/3} \hat{\mathbf{F}} \quad ; \quad \hat{\mathbf{C}} = J^{-2/3} \mathbf{C} = \hat{\mathbf{F}}^T \hat{\mathbf{F}} \quad (2.6)$$

into its two constituents; i.e., *pure dilatation*, $J^{1/3} \mathbf{I}$, and *isochoric distortional* deformation, $\hat{\mathbf{F}}$ ($\det \hat{\mathbf{F}} = 1$). Correspondingly, we refer to the Lagrangian tensor $\hat{\mathbf{C}}$ as the *modified*, volume-preserving, deformation tensor. This provides for a proper treatment of uncoupled volumetric/deviatoric response of, for example, incompressible rubbers [5,8,13].

Considering the second of Eqs. (2.6), the (directional) derivative formula [14,15] for $\hat{\mathbf{C}}$ leads to:

$$D\hat{\mathbf{C}} \cdot \mathbf{A} = J^{-2/3} \left[\mathbf{A} - \frac{1}{3} (\mathbf{C}^{-1} : \mathbf{A}) \mathbf{C} \right] \quad (2.7a)$$

for any variation \mathbf{A} in tensor \mathbf{C} , and we thus have

$$\partial \hat{\mathbf{C}} / \partial \mathbf{C} = J^{-2/3} \left[\mathbf{I}^{(4)} - \frac{1}{3} \mathbf{C} \otimes \mathbf{C}^{-1} \right] \quad (2.7b)$$

where symbols $:$ and \otimes denote *scalar* multiplication (i.e., trace operation) and *vector* product of tensors, respectively; and the components of the fourth-order, symmetric, *unit* tensor $\mathbf{I}^{(4)}$ is given by

$$I_{ijkl}^{(4)} = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \quad (2.8)$$

2.2 Material (Convected) and Spatial Description

The geometric notions of “pull-back” and “push-forward” operations for tensor and vector fields on manifolds [15] play an important role in developing “counterpart” expressions for the stress-deformation and material-moduli (elasticity) tensors in both *material* (Lagrangian) and *spatial* (Eulerian) settings. They provide the appropriate forms in finite element formulations based on total and updated Lagrange methods, respectively [8,20].

Proper definitions of these operations require identification of the precise placement of tensor indices (i.e., "covariant" or "contravariant" components), even in a rectangular Cartesian setting. Therefore, considering the case of "contravariant" tensor (vector) fields that are (independently) defined on various configurations, and letting \mathbf{T} be a second-order material tensor field defined on "B", its push-forward $\phi_* \mathbf{T}$ is a spatial tensor, \mathbf{T}' , of the same contravariant type on "b", or $\phi(\mathbf{B})$, which is given by

$$\mathbf{T}' \equiv \phi_* \mathbf{T} = \mathbf{F} \mathbf{T} \mathbf{F}^T \quad (2.9)$$

Alternatively, letting \mathbf{t} be a "contravariant" two-tensor field on "b", its pull-back, \mathbf{t}' , on "B" is defined as

$$\mathbf{t}' \equiv \phi^* \mathbf{t} = \mathbf{F}^{-1} \mathbf{t} \mathbf{F}^T \quad (2.10)$$

As an application of this latter operation, we recall here that the (symmetric) *second Piola-Kirchhoff* stress \mathbf{S} is actually the pull-back of the Kirchhoff stress $\boldsymbol{\tau} = \mathbf{J} \boldsymbol{\sigma}$ (where $\boldsymbol{\sigma}$ is the *Cauchy* or true stress tensor); i.e.,

$$\mathbf{S} \equiv \phi^* \boldsymbol{\tau} = \mathbf{F}^{-1} \boldsymbol{\tau} \mathbf{F}^T \quad (2.11)$$

Similarly, considering the (covariant) components of the material and spatial strain tensors \mathbf{E} and \mathbf{e} , we have

$$\mathbf{e} = \phi_* \mathbf{E} = \mathbf{F}^T \mathbf{E} \mathbf{F}^{-1} \quad (2.12)$$

Finally, we note that the above notions are also useful for deriving different forms for *objective* rates for spatial stress and strain fields [14-16]. For example, we cite here the two most commonly used rates of this type; i.e., the Truesdell rate of Cauchy stress, $\overset{\circ}{\boldsymbol{\sigma}}$, and the rate of deformation tensor, \mathbf{d} (time, and an overdot signifies a material time derivative):

$$\overset{\circ}{\boldsymbol{\sigma}} = \frac{1}{J} \phi_* \left[\frac{\partial}{\partial t} (\phi^* \boldsymbol{\tau}) \right] = \frac{1}{J} \mathbf{F} \dot{\mathbf{S}} \mathbf{F}^T \quad (2.13)$$

$$\mathbf{d} = \phi_* \left[\frac{\partial}{\partial t} (\phi^* \mathbf{e}) \right] = \mathbf{F}^T \dot{\mathbf{E}} \mathbf{F}^{-1} \quad (2.14)$$

In view of the above equations, we actually proceed for the remainder of the paper with derivations in terms of the material-type tensors \mathbf{S} and \mathbf{E} and the associated rates; i.e., for the stress-deformation relations and material-moduli (fourth-order) tensors \mathbf{D} (recall Eq. 2.4):

$$S = S(C) \quad ; \quad \dot{S} = D(C)\dot{E} \quad (2.15)$$

where () indicates "a function of". The "counterpart" spatial forms follow directly by the push-forward/pull-back according to Eqs. (2.11) to (2.14). In particular, for the spatial tensor \bar{D} one has

$$J\delta = \bar{D}(e)d \quad ; \quad J\bar{D} = F_{im}F_{jn}D_{mnpq}(\bar{C})F_{kp}F_{lq} \quad (2.16)$$

2.3 Spectral Representation

Denoting by λ_i and \mathbf{n}_i ($i = 1,2,3$) the principal values of \mathbf{C} (i.e., *square* of principal stretches) and their associated eigenvectors, respectively, we can utilize the following representation for its components:

$$\mathbf{C} = \sum_{i=1}^3 \lambda_i (\mathbf{n}_i \otimes \mathbf{n}_i) = \sum_{i=1}^3 \lambda_i \mathbf{N}_i \quad (2.17)$$

or, equivalently, in terms of the (rank-one) 3x3 matrices \mathbf{N}_i ,

(i) for the case of *distinct* λ_i :

$$\mathbf{C} = \sum_{i=1}^3 \lambda_i \mathbf{N}_i \quad (2.18a)$$

(ii) for the case of *double coalescence* ($\lambda_r \neq \lambda_s = \lambda_t = \lambda$):

$$\mathbf{C} = (\lambda_r - \lambda) \mathbf{N}_r + \lambda \mathbf{I} \quad (2.18b)$$

(iii) for the case of *triple coalescence* ($\lambda_1 = \lambda_2 = \lambda_3 = \lambda$):

$$\mathbf{C} = \lambda \sum_{i=1}^3 \mathbf{N}_i = \lambda \mathbf{I} \quad (2.18c)$$

In the above, the (r,s,t) is any *cyclic* permutation of (1,2,3), and tensors \mathbf{N}_i are often referred to as the (orthogonal) *eigenprojection* operators (i.e., on the null space of $\mathbf{C} - \lambda_i \mathbf{I}$); e.g., see [18,19] for further details. Note that, among the latter tensors, only those which are uniquely defined (i.e., corresponding to *distinct* eigenvalues) are employed in Eqs. (2.18).

Explicit expressions for N_i in terms of \mathbf{C} can be obtained by suitable manipulations of Eqs. (2.18).

This leads to the following forms corresponding to previous cases (i) and (ii):

$$(i) \quad N_r = \frac{1}{(\lambda_r - \lambda_s)(\lambda_s - \lambda_t)} \left[(C - \lambda_s I)(C - \lambda_t I) \right] \quad (2.19a)$$

$$(ii) \quad N_r = \frac{1}{(\lambda_r - \lambda)} (C - \lambda I) \quad (2.19b)$$

These will prove very useful in obtaining the derivatives of the stress function $\mathbf{S} = \mathbf{S}(\mathbf{C})$ in Secs. 5 and 6.

Remark 2.1. Alternatively, following standard procedures: e.g. as outlined in [17, p. 563], we can show that

$$(\lambda_r - \lambda_s)(\lambda_r - \lambda_t) N_r = \text{Cof} (C - \lambda_r I)$$

where $\text{Cof} (\cdot)$ denotes the adjoint matrix whose elements are the *cofactors* of (\cdot) ; i.e., with its $(i,j)^{\text{th}}$ component given by

$$\frac{1}{2} \varepsilon_{mpi} \varepsilon_{nqj} (C_{mn} - \lambda_r \delta_{mn}) (C_{pq} - \lambda_r \delta_{pq})$$

where ε is the rank-three alternating tensor. Together with the identity:

$$\varepsilon_{ijk} \varepsilon_{lmn} = \delta_{il} \delta_{jm} \delta_{kn} + \delta_{im} \delta_{kl} \delta_{jn} + \delta_{in} \delta_{jl} \delta_{km} - (\delta_{il} \delta_{km} \delta_{jn} + \delta_{im} \delta_{jl} \delta_{kn} + \delta_{in} \delta_{kl} \delta_{jm})$$

this Cof tensor can be simplified to exactly the same form in the bracketed term on the right-hand side of Eq. (2.19).

3. STRESS-DEFORMATION RELATIONS, THE SEPARABLE AND UNCOUPLED VOLUMETRIC/DEVIATORIC FORMS FOR STRAIN ENERGY FUNCTION

Restricting attention to the hyperelastic *isotropic* material case, the two forms of the strain-energy function, W , considered here are written as:

$$W \equiv W(\lambda_i) = \sum_{n=1}^N a_n (\lambda_1^{\alpha_n} + \lambda_2^{\alpha_n} + \lambda_3^{\alpha_n}) \quad (3.1)$$

and

$$W = \hat{W}(\hat{\lambda}_i) + h(J) \quad (3.2)$$

where λ are the principal values of $\hat{\mathbf{C}}$ (see Eq. 2.6); h is a (convex) function of one variable $J = (\lambda_1 \lambda_2 \lambda_3)^{1/2}$, and the a_n and α_n are material constants. The functional dependence of \hat{W} in Eq. (3.2) is assumed

to be exactly in the *same separable* form as in Eq. (3.1), but with the modified stretches $\hat{\lambda}_i$ now replacing λ_i (where $\hat{\lambda}_i = J^{-2/3} \lambda_i$ from Eq. 2.6).

Note that in most practical applications, the $h(J)$ is actually taken as a *penalty* function imposing the incompressibility (or rather, the slight-compressibility) constraint [5,6,8,11,12]. In this connection, we also note that an implicit assumption of strict incompressibility is often made [5,6] when using Eq. (3.1). However, such an assumption is *not* implied here, and for emphasis we refer to this material model as the *unconstrained* general case. Of course, adding a penalty-like term for the purpose of practical usage is the same as for Eq. (3.2). However, the separate treatment of Eq. (3.1) will provide the basis for subsequent derivations of the **D** tensor in the more complex situation of Eq. (3.2).

The constitutive functions $\mathbf{S} = \mathbf{S}(\mathbf{C})$ and $\mathbf{D} = \mathbf{D}(\mathbf{C})$ can now be obtained

$$\mathbf{S} = 2 \frac{\partial W}{\partial \mathbf{C}} \quad ; \quad \mathbf{D} = 4 \frac{\partial^2 W}{\partial \mathbf{C} \partial \mathbf{C}} \quad (3.3)$$

or

$$\mathbf{S} = 2 \left[\frac{\partial \hat{W}}{\partial \hat{\mathbf{C}}} \frac{\partial \hat{\mathbf{C}}}{\partial \mathbf{C}} + h' \frac{\partial J}{\partial \mathbf{C}} \right] \quad ; \quad \mathbf{D} = 2 \frac{\partial \mathbf{S}}{\partial \mathbf{C}} \quad (3.4)$$

where the primes denote differentiation of h with respect to its argument, J . Together with Eq. (2.7), the expression in Eq. (3.4) can be reduced to

$$\mathbf{S} = J^{-2/3} \text{DEV} \left(2 \frac{\partial \hat{W}}{\partial \hat{\mathbf{C}}} \right) + p J \mathbf{C}^{-1} \quad (3.5a)$$

with

$$\text{DEV}(\mathbf{B}) = \mathbf{B} - \frac{1}{3} (\mathbf{B} : \mathbf{C}) \mathbf{C}^{-1} \quad (3.5b)$$

for any Lagrangian (stress-type) variation tensor \mathbf{B} , and where $p = h'$ is the (hydrostatic) pressure function. The DEV operator in Eq. (3.5b) allows for a concise writing of several expressions given later; physically it gives the *deviatoric* part of the *material* tensor \mathbf{A} , see Sec 5.2. Its *spatial* counterpart: e.g. $\text{dev } \underline{\underline{\sigma}} = \underline{\underline{\sigma}} - \frac{1}{3} \text{tr}(\underline{\underline{\sigma}}) \mathbf{I}$, where $\text{tr}(\cdot)$ indicates the trace of (\cdot) , is an already well-known operation.

4. MATERIAL-MODULI TENSOR. THE GENERAL UNRESTRAINED MODEL

4.1 Continuous Representation of the Constitutive Stress Function

We start by first considering the case of Eqs. (3.1) and (3.3). Making use of the fact that, for the present isotropic material, \mathbf{S} is *coaxial* with \mathbf{C} (i.e., identical eigenvectors for both), it admits a representation in terms of its principal values S_i ($i = 1,2,3$), and directions \mathbf{N}_i (Eq. 2.19), in exactly the same form as in Eqs. (2.18). Explicitly, for the present separable W-form in Eq. (3.1), we have

$$S_i = 2W_{,i} = 2 \sum_{n=1}^N \alpha_n a_n \lambda_i^{\alpha_n-1} \equiv S(\lambda_i) \quad (4.1)$$

i.e. the *same* functional dependence S on only λ_i , for each separate $i = 1,2,3$, where a comma-subscript with W indicates (partial) differentiation with respect to (w.r.t.) the following principal-stretch "coordinate". Combining Eqs. (2.18, 2.19), and (4.1) leads to

$$(i) \quad \mathbf{S} = a \mathbf{C}^2 + b \mathbf{C} + c \mathbf{I} \quad (4.2a)$$

$$(ii) \quad \mathbf{S} = \bar{a} \mathbf{C} + \bar{b} \mathbf{I} \quad (4.2b)$$

$$(iii) \quad \mathbf{S} = S(\lambda) \mathbf{I} \quad (4.2c)$$

where (i)-(iii) correspond to the three cases considered previously in Eq. (2.18), and

$$a = - \sum_{r=1}^3 m(\lambda_r - \lambda_s) S(\lambda_r) \quad (4.3a)$$

$$b = \sum_{r=1}^3 m(\lambda_r^2 - \lambda_s^2) S(\lambda_r) \quad (4.3b)$$

$$c = - \sum_{r=1}^3 m(\lambda_r - \lambda_s) \lambda_r \lambda_s S(\lambda_r) \quad (4.3c)$$

$$m = \frac{1}{(\lambda_1 - \lambda_2)(\lambda_2 - \lambda_3)(\lambda_3 - \lambda_1)} \quad (4.3d)$$

$$\bar{a} = [S(\lambda_r) - S(\lambda)] / (\lambda_r - \lambda) \quad (4.4a)$$

$$\bar{b} = - \left[\lambda S(\lambda_r) - \lambda_r S(\lambda) \right] / (\lambda_r - \lambda) \quad (4.4b)$$

Recall that the (r,s,t) are still cyclic permutations of (1,2,3), and all notations follow those used previously in Eqs. (2.18).

With the above expressions, one can easily proceed to investigate the *continuity* of the functional representation of $\mathbf{S} = \mathbf{S}(\mathbf{C})$. In fact, this simply amounts to showing that the limits for Eq. (4.2a) exist, and that these are given by Eqs. (4.2b) and (4.2c) when the *distinct* eigenvalues $(\lambda_r, \lambda_s, \lambda_t)$ approach $(\lambda_r, \lambda, \lambda)$ and $(\lambda, \lambda, \lambda)$, respectively. For example, considering the former case, we let $\underline{\lambda} = (\lambda_r, \lambda_s, \lambda_t) \rightarrow \bar{\lambda} = (\lambda_r, \lambda, \lambda)$ along the *line* normal to the plane $\lambda_s = \lambda_t$, and there results, for the limits of $a(\lambda)$, $b(\lambda)$, etc.

$$\lim_{\underline{\lambda} \rightarrow \bar{\lambda}} a = \frac{1}{(\lambda_r - \lambda)^2} [S(\lambda_r) - S(\lambda) - (\lambda_r - \lambda) S'(\lambda)] \quad (4.5a)$$

$$\lim_{\underline{\lambda} \rightarrow \bar{\lambda}} b = \frac{1}{(\lambda_r - \lambda)^2} \left\{ (\lambda_r^2 - \lambda^2) S'(\lambda) - 2\lambda [S(\lambda_r) - S(\lambda)] \right\} \quad (4.5b)$$

$$\lim_{\underline{\lambda} \rightarrow \bar{\lambda}} c = \frac{1}{(\lambda_r - \lambda)^2} \left[\lambda^2 S(\lambda_r) + \lambda_r(\lambda_r - 2\lambda) S(\lambda) - \lambda_r \lambda (\lambda_r - \lambda) S'(\lambda) \right] \quad (4.5c)$$

$$\lim_{\underline{\lambda} \rightarrow \bar{\lambda}} C^2(\lambda) = \frac{1}{(\lambda_r - \lambda)} \left[(\lambda_r^2 - \lambda^2) C(\bar{\lambda}) - (\lambda \lambda_r^2 - \lambda^2 \lambda_r) \mathbf{I} \right] \quad (4.5d)$$

Recall that a prime indicates differentiation w.r.t. the shown (single) argument. Substituting Eqs. (4.5) into (4.2a), we obtain the expression in (4.2b).

Similar arguments can be used for the case of triple coalescence, by finding the limits of \mathbf{S} in Eq. (4.2a) when distinct $\lambda = (\lambda_r, \lambda_s, \lambda_t) \rightarrow \bar{\lambda} = (\lambda, \lambda, \lambda)$ along the *line* normal to the principal space diagonal, or hydrostatic axis [e.g., 17], $\lambda_r = \lambda_s = \lambda_t$. The result is expression (4.2c).

Remark 4.1. Based on available results from strict mathematical analyses; i.e., the so-called Ball's Lemma [28], the continuous *differentiability* of any tensor-valued function like $\mathbf{S} = \mathbf{S}(\mathbf{C})$; e.g. its elastic moduli-tensor \mathbf{D} of concern here (see Eq. 3.3), is guaranteed if we can simply show that the limits of $\mathbf{D}(\underline{\lambda})$ with distinct $\underline{\lambda} = (\lambda_r, \lambda_s, \lambda_t)$ exist for the "degenerate" cases when $\underline{\lambda} \rightarrow (\lambda_r, \lambda, \lambda)$ or $\underline{\lambda} \rightarrow (\lambda, \lambda, \lambda)$ along the two lines that are normal to the plane $\lambda_s = \lambda_t$, and to the line $\lambda_r = \lambda_s = \lambda_t$, following similar arguments as the above.

The presence of an *individual* λ_r -argument for each $S(\lambda_r)$ -function in various terms of $\mathbf{D}(\mathbf{C})$ will provide for considerable simplifications here.

4.2 Explicit Expressions for \mathbf{D}

The general expression for tensor \mathbf{D} can be obtained by applying the directional derivative formula to Eq. (4.2a), recalling the second of Eqs. (3.4), and making use of the formula $\partial\lambda_r/\partial C = N_r$ (see Eq. 2.17) for the present case (i) of *distinct* λ_i ($i=1,2,3$). Although tedious, it is straight-forward to show that

$$\begin{aligned} (i) \quad \mathbf{D} = & a_1 \mathbf{P}(\mathbf{C}^2, \mathbf{C}^2) + a_2 [\mathbf{P}(\mathbf{C}^2, \mathbf{C}) + \mathbf{P}(\mathbf{C}, \mathbf{C}^2)] \\ & + a_3 [\mathbf{Q}(\mathbf{C}^2, \mathbf{I}) + \mathbf{Q}(\mathbf{I}, \mathbf{C}^2)] + a_4 \mathbf{P}(\mathbf{C}, \mathbf{C}) \\ & + a_5 [\mathbf{Q}(\mathbf{C}, \mathbf{I}) + \mathbf{Q}(\mathbf{I}, \mathbf{C})] + 2a_6 \mathbf{I}^{(4)} \end{aligned} \quad (4.6a)$$

where we define, for any two (second-order-symmetric-tensor) arguments \mathbf{G}, \mathbf{H} , the components of the fourth-order tensors, \mathbf{P} and \mathbf{Q} , as

$$P_{ijkl}(\mathbf{G}, \mathbf{H}) = G_{ik} H_{jl} + G_{il} H_{jk} \quad (4.6b)$$

$$Q_{ijkl}(\mathbf{G}, \mathbf{H}) = G_{ik} H_{jl} + G_{il} H_{jk} + G_{jk} H_{il} + G_{jl} H_{ik} \quad (4.6c)$$

and $\mathbf{I}^{(4)}$ is given in Eq. (2.8). We have also utilized the following definitions for scalar coefficients

a_i ($i=1 \rightarrow 6$):

$$a_1 = \sum_{r=1}^3 \eta_r \quad ; \quad a_2 = \sum_{r=1}^3 (\lambda_r - I_1) \eta_r \quad ; \quad a_3 = \sum_{r=1}^3 I_3 \eta_r / \lambda_r \quad (4.6d)$$

$$a_4 = \sum_{r=1}^3 (I_1 - \lambda_r)^2 \eta_r \quad ; \quad a_5 = \sum_{r=1}^3 \mu_r + I_3 \eta_r (\lambda_r - I_1) / \lambda_r \quad (4.6e)$$

$$a_6 = \sum_{r=1}^3 \eta_r (I_3 / \lambda_r)^2 + (\lambda_r - I_1) \mu_r \quad (4.6f)$$

in which

$$I_1 = \lambda_1 + \lambda_2 + \lambda_3 \quad ; \quad I_2 = \lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_3\lambda_1 \quad ; \quad I_3 = \lambda_1\lambda_2\lambda_3 \quad (4.6g)$$

$$\eta_r = \left[S'(\lambda_r) + (\lambda_s - \lambda_r) (\mu_r + \mu_t) + (\lambda_t - \lambda_r) (\mu_r + \mu_s) \right] / \left[(\lambda_r - \lambda_s)^2 (\lambda_r - \lambda_t)^2 \right] \quad (4.6h)$$

$$\mu_r = S(\lambda_r) / [(\lambda_r - \lambda_s)(\lambda_r - \lambda_t)] \quad (4.6i)$$

where the principal values $S(\lambda_r)$ and their derivatives w.r.t. λ_r , $S'(\lambda_r)$, are found from Eqs. (4.1), and the (r,s,t) is again any cyclic permutation of $(1,2,3)$.

Considering now the two degenerate cases (ii) and (iii) of double and triple coalescence of λ_i values, respectively (Eq. 2.18), we proceed in exactly the same manner as in Sec. 4.1 to find the associated limits of the expression in Eqs. (4.6). Omitting all the details and considerable simplifications involved, we summarize the results as follows:

$$(ii) \quad \mathbf{D} = b_1 \mathbf{P}(\mathbf{C}, \mathbf{C}) + b_2 [\mathbf{Q}(\mathbf{C}, \mathbf{I}) + \mathbf{Q}(\mathbf{I}, \mathbf{C})] + 2b_3 \mathbf{I}^{(4)} \quad (4.7)$$

$$(iii) \quad \mathbf{D} = 2S'(\lambda) \mathbf{I}^{(4)} \quad (4.8)$$

where

$$b_1 = \alpha \left\{ (\lambda_r - \lambda) \left[S'(\lambda_r) + S'(\lambda) \right] - 2 \left[S(\lambda_r) - S(\lambda) \right] \right\} \quad (4.9a)$$

$$b_2 = \alpha \left\{ (\lambda - \lambda_r) \left[\lambda S'(\lambda_r) + \lambda_r S'(\lambda) \right] + (\lambda_r + \lambda) \left[S(\lambda_r) - S(\lambda) \right] \right\} \quad (4.9b)$$

$$b_3 = \alpha \left\{ (\lambda_r - \lambda) \left[\lambda_r^2 S'(\lambda) + \lambda^2 S'(\lambda_r) \right] - 2\lambda_r \lambda \left[S(\lambda_r) - S(\lambda) \right] \right\} \quad (4.9c)$$

$$\alpha = 1/(\lambda_r - \lambda)^3 \quad (4.9d)$$

Remark 4.2. (i) All formulas in Eqs. (4.6) - (4.8) exhibit proper symmetries in the \mathbf{D} arrays; i.e., with symmetric strain rates $\dot{\mathbf{E}}$ (and $\dot{\mathbf{C}}$), and stress rate $\dot{\mathbf{S}}$ tensors (see Eq. 2.15), $D_{ijkl} = 1/2 (\partial S_{ij} / \partial C_{kl} + \partial S_{ij} / \partial C_{lk})$. (ii) In view of the existence of the collective limits in Eqs. (4.7) and (4.8), the continuous differentiability of \mathbf{D} follows immediately from results in [28] (although this is *not* true for the constituent arguments, and λ_i and \mathbf{N}_i of \mathbf{C}). (iii) Restricting the dimension of the underlying space of all tensors in Eqs. (4.6) - (4.8) to two, it can be shown that the \mathbf{D} arrays corresponding to the general distinct-eigenvalues case (e.g., $\lambda_1 = \lambda_r \neq \lambda_2 = \lambda$) and the repeated-two-eigenvalues case (i.e., $\lambda_1 = \lambda_2 = \lambda$) are actually those in Eqs. (4.7) and (4.8), respectively; *no* separate treatment is therefore necessary for this *two-dimensional* problem.

Remark 4.3. Being also *coaxial* with \mathbf{C} , the logarithmic strain, $\ln \mathbf{U} = \sum_{r=1}^3 (\ln \lambda_r^{1/2}) \mathbf{N}_r$, for distinct λ_r , can be treated similar to the present case; i.e., its (material) time derivative takes the forms of Eqs. (4.6) - (4.8), except now its principal values (in parenthesis in the above summation) replace $S(\lambda_r)$. This may prove useful in, for example, large-strain elastoplastic finite element applications as in [e.g. 27]. We also

note that the present formulas for the spectral representations of "coaxial" *tensor-valued* functions (e.g. **S** here), and their derivatives, in terms of the *argument tensor* (e.g. **C** here), will prove very useful in applications involving continuum-based *damage* constitutive models and the experimental characterization of material coefficients, e.g. see [30].

5. MATERIAL-MODULI TENSOR. THE UNCOUPLED VOLUMETRIC/DEVIATORIC MODEL

The analysis in the present case proceeds parallel to that given in the previous section. We therefore draw extensively on the results of Sec. 4 and omit many details.

5.1 Continuous Representation of the Constitutive Stress Function

In view of the *coaxiality* of tensor **C**, **S**, and $\hat{\mathbf{C}}$, and making use of Eq. (3.2) to explicitly evaluate the term DEV in Eq. (3.5), one can conveniently write the stress function in the present case as:

$$\mathbf{S} = J^{-2/3} \hat{\mathbf{S}} + f(\hat{\lambda}_i) \mathbf{C}^{-1} + p J \mathbf{C}^{-1} \quad (5.1a)$$

with

$$\hat{\mathbf{S}} = 2\partial\hat{W}/\partial\hat{\mathbf{C}} \quad ; \quad \hat{S}_r = 2\hat{W}_{,r} = \hat{S}(\hat{\lambda}_r) \quad (5.1b)$$

$$f(\hat{\lambda}_i) = -\frac{2}{3} \sum_{r=1}^3 \hat{\lambda}_i \hat{W}_{,r} \quad (5.1c)$$

In this, the \hat{S}_r ($r=1,2,3$) are the principal values of $\hat{\mathbf{S}}$, and the comma subscript in \hat{W} defines differentiation w.r.t. *modified* parameters $\hat{\lambda}$. We make the important observation that, with Eq. (3.2), the \hat{S}_r displays exactly the same *symmetric-single argument* dependence as in Eq. (4.1); i.e., $\hat{\mathbf{S}}$ admits the same limiting forms as in Eqs. (4.2) in terms of $\hat{\mathbf{C}}$.

With the neat separation of its constituents, no further elaboration is actually needed regarding the representation of **S** in Eq. (5.1a). The last two terms on the right-hand side are always well-behaved for any λ_i , whereas the continuity of $\hat{\mathbf{S}}$ for distinct as well as repeated λ_i follows immediately from the analysis in Sec. 4 (simply replace λ_i by $\hat{\lambda}_i$, **C** by $\hat{\mathbf{C}}$, and **S** by $\hat{\mathbf{S}}$ in pertinent paragraphs). Note that this will also be the case for constituents of the **D** tensor given in the sequel.

5.2 Explicit Expressions for **D**

A careful examination of the derivatives of various terms in Eq. (5.1a) w.r.t. components **C** reveals that, for all cases (i.e., distinct as well as repeated eigenvalues), a single general expression can be written

for \mathbf{D} ; some of the terms will, however, need to be "branched out" for their individual explicit evaluation.

That is

$$\mathbf{D} = J^{-2/3} \mathbf{D}\hat{\mathbf{S}} + \mathbf{Y} + (p''J + p'J^2) \mathbf{C}^{-1} \otimes \mathbf{C}^{-1} - \frac{2}{3} \hat{\mathbf{S}} \otimes \hat{\mathbf{C}}^{-1} + 2\hat{\mathbf{C}}^{-1} \otimes \text{DEV}(\mathbf{M}) \quad (5.2a)$$

in which

$$\mathbf{Y} = - \left[pJ + f(\hat{\lambda}_i) \right] \mathbf{P} (\mathbf{C}^{-1}, \mathbf{C}^{-1}) \quad (5.2b)$$

where the primes in p' and p'' indicate first and second derivatives, respectively, w.r.t. J , the tensor operator \mathbf{P} is defined as in Eq. (4.6b), and the newly-introduced tensors $\mathbf{D}\hat{\mathbf{S}}$ (fourth-order) and \mathbf{M} (second-order) are defined by

$$\mathbf{D}\hat{\mathbf{S}} \equiv 2\partial\hat{\mathbf{S}}/\partial\mathbf{C} = J^{-2/3} \mathbf{A} - \frac{2}{3} \mathbf{B} \otimes \hat{\mathbf{C}}^{-1} \quad (5.2c)$$

$$\mathbf{M} \equiv \partial f(\hat{\lambda}_i)/\partial\hat{\mathbf{C}} = \mathbf{M}(\hat{\mathbf{C}}) \quad (5.2d)$$

The above decompositions in formulas (5.2c) and (5.2d) are made to facilitate the use of previous expressions; namely, by its definition the (fourth-order) tensor $\mathbf{A} = \mathbf{A}(\mathbf{C})$ is obtained in exactly the same manner as was for $\mathbf{D}(\mathbf{C})$ in case of the unconstrained model of Sec. 4. Thus, using the following replacements (assignment "operators"):

$$\hat{\mathbf{C}} \leftarrow \mathbf{C} \quad ; \quad \hat{\lambda}_i \leftarrow \lambda_i \quad ; \quad \hat{\mathbf{S}}(\hat{\lambda}) \leftarrow \mathbf{S}(\lambda) \quad (5.3a)$$

and

$$a_i(\hat{\lambda}_r) \leftarrow a_i(\lambda_r) \text{ for } i = 1 \text{ to } 6 \quad (5.3b)$$

$$b_i(\hat{\lambda}_r) \leftarrow b_i(\lambda_r) \text{ for } i = 1 \text{ to } 3 \quad (5.3c)$$

we can now write

$$(i) \mathbf{A} = \text{Eq. (4.6)} ; (ii) \mathbf{A} = \text{Eq. (4.7)} ; (iii) \mathbf{A} = \text{Eq. (4.8)} \quad (5.4)$$

Similarly, we can use the above assignments in finding the scalar product of \mathbf{A} and $\hat{\mathbf{C}}$ needed in the last term of Eq. (5.2c); see the scalar operator $\mathbf{C}^{-1}:\mathbf{A}$ of Eq. (2.7a). There results, for the (second-order) tensor \mathbf{B} , and upon use of the Cayley-Hamilton theorem [14,15],

$$\mathbf{B}^{(m)} = q_1^{(m)} \hat{\mathbf{C}}^2 + q_2^{(m)} \hat{\mathbf{C}} + q_3^{(m)} \mathbf{I} \quad ; \quad \text{for } m = \text{(i) or (ii)} \quad (5.5)$$

$$\mathbf{B}^{(iii)} = \hat{S}(\hat{\lambda}) \hat{\mathbf{C}} \quad (5.6)$$

where for Case (i):

$$q_1 = [\hat{I}_1(\hat{I}_1^2 - 2\hat{I}_2) + \hat{I}_3] a_1 + 2(\hat{I}_1^2 - \hat{I}_2) a_2 + \hat{I}_1(2a_3 + a_4) + 2a_5 \quad (5.7a)$$

$$q_2 = (\hat{I}_1\hat{I}_3 + \hat{I}_2^2 - \hat{I}_1^2\hat{I}_2) a_1 + 2(\hat{I}_3 - \hat{I}_1\hat{I}_2) a_2 - \hat{I}_2(2a_3 + a_4) + a_6 \quad (5.7b)$$

$$q_3 = \hat{I}_3(\hat{I}_1^2 - \hat{I}_2) a_1 + 2\hat{I}_1\hat{I}_3 a_2 + \hat{I}_3(2a_3 + a_4) \quad (5.8a)$$

and for Case (ii):

$$q_1 = \hat{I}_1 b_1 + 2b_2 \quad ; \quad q_2 = b_3 - b_1 \hat{I}_2 \quad ; \quad q_3 = b_1 \hat{I}_3 \quad (5.8b)$$

On the other hand, considering the definition of tensor \mathbf{M} in Eq. (5.2d), its functional dependence on $\hat{\mathbf{C}}$ is of the same form as that of \mathbf{S} in Eqs. (4.2) – (4.4) in terms of \mathbf{C} for the unconstrained model. Thus, invoking the assignment “equations” (5.3), together with $M(\hat{\lambda}_i) \leftarrow S(\lambda_i)$, we can write

$$\text{(i) } \mathbf{M} = \text{Eq. (4.2a)} \quad ; \quad \text{(ii) } \mathbf{M} = \text{Eq. (4.2b)} \quad ; \quad \text{(iii) } \mathbf{M} = \text{Eq. (4.2c)} \quad (5.9)$$

where the principal values $M_i = M(\hat{\lambda}_i)$ are given by (recall Eq. 5.1c)

$$M(\hat{\lambda}_i) = -\frac{2}{3}(\lambda \hat{W}_{,ii} + \hat{W}_{,i}) \quad (5.10)$$

Finally, by virtue of the continuity of the “new” tensors \mathbf{A} , \mathbf{B} , $\hat{\mathbf{S}}$, and \mathbf{M} in terms of $\hat{\mathbf{C}}$, and according to the previous analysis in Sec. 4, the expression for \mathbf{D} in Eq. (5.2) is, ensured to be “well-defined” for the entire range of λ_i .

Remark 5.1. In implementation, one actually uses $\mathbf{C}^{-1} = (\mathbf{C}^2 - \mathbf{I}_1 \mathbf{C} + \mathbf{I}_2 \mathbf{I})/\mathbf{I}_3$. Also, explicit expressions are available for λ_i and $\hat{\lambda}_i$ directly in terms of \mathbf{C} ; e.g. using the $(\mathbf{I}_1, \mathbf{I}_2, \theta)$ set of invariants; see [17, p. 269] for details.

6. COMPARISON WITH AVAILABLE RESULTS

By way of a simple illustration, we compare some of the expressions obtained here with those available for the *two-dimensional* case in [e.g. 8]. To this end, we consider the case of (two-dimensional) double coalescence, and recollect the final observation (iii) made in Remark 4.2. Thus, for the model of Sec. 4, we simply use Eq. (4.8) here; i.e., with $g = W_{,rr}$ (same for any r), $\mathbf{D} = 4 g \mathbf{I}^{(4)}$, which, despite its extreme simplicity, leads to exactly the same coefficients; e.g., $D_{1111} = 4g$, $D_{1122} = 0$, and $D_{1212} = D_{1221} = 2g$, etc., as those derived differently in [8,13].

Similarly, although not included here to limit the space, the detailed term-by-term expansions for \mathbf{D} have also confirmed the equivalence of the forms given in [8,13], for the general two-dimensional case with distinct eigenvalues, to those obtained from Eq. (4.7) in the present three-dimensional case with double coalescence (with appropriate restrictions of the range of subscripts in \mathbf{S} , \mathbf{C} , \mathbf{E} , etc.). Of course, modifications should be made in these comparisons to allow for different notations and definitions used (e.g. the engineering definition for shear strains in \mathbf{E} instead of the tensorial ones employed here, etc.).

7. CONCLUSIONS

Taken separately, the main constituents of the deformation tensor, i.e., principal values and associated eigenvectors, are, in general, not uniquely-defined and continuously differentiable functions. A careful consideration is thus called for in implementing constitutive models formulated in terms of these principal-strain measures, and this is the main problem addressed in this paper. In particular, the difficulty is entirely bypassed by resorting to explicit derivations of appropriate forms of the material tangent-stiffness matrices which are valid for the entire deformation range. These were developed here for two specific forms of the Ogden-type, strain-energy functions, which actually encompass many of the popular representations currently in use for rubber materials. A key feature in these is the underlying separability property, and this was employed to obtain the concise final forms of the tensor expressions, thus leading to their effective and robust numerical implementation.

In view of the results obtained, it became obvious that the task simply amounts to application of a systematic limiting procedure for only one type of tensor-valued functions and their material time derivatives; i.e., those with symmetric single-argument functions in their spectral representation. In

particular, this was found essential in greatly simplifying the development given for the important case of uncoupled volumetric/deviatoric formulations. Finally, an important area for effective utilization of the present results would be to explore the feasibility of systematically deriving the *full* expanded forms, together with generating the associated computer codes for implementation, using computer symbolic-manipulation packages [29].

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